CRD report

News from the LBNL Computational Research Division

September 2005

Latest Version of IMG Genome Analysis Tool Released

DOE has released an enhanced version of the Integrated Microbial Genomes (IMG) data management system jointly developed by the Biological Data Management and Technology Center (BDMTC) in CRD and the Joint Genome Institute (JGI). The new version, IMG 1.2, contains 270 additional public genomes and nine (four finished, five draft) new JGI genomes, bringing the total number of genomes in IMG to 618 (318 bacterial, 25 archaeal, 15 eukaryotic, 260 bacterial phage), 40 of which are finished and 80 of which are draft genomes sequenced by DOE's JGI.

IMG 1.2 enables users to add annotations to IMG as well as to save the results of their analysis of organisms and genes. IMG 1.2 also features enhanced comparative analysis capabilities.

Since its initial release in March 2005, IMG has gained increasing recognition in the scientific community. "IMG is invaluable for comparative genomic analyses," said Mark A. Schell, professor in the Department of Microbiology and Plant Pathology at the University of Georgia. "My laboratory uses it all the time and I will use it in the classes I teach this fall."

Developed as a community resource, IMG will integrate JGI's microbial genome data with publicly available microbial genome data, and thus provide a powerful comparative context for microbial genome analysis.

The BDMTC, headed by Victor Markowitz, was established in January 2004 to serve as a source of expertise in and provide

(continued on page 2)

CRD Report

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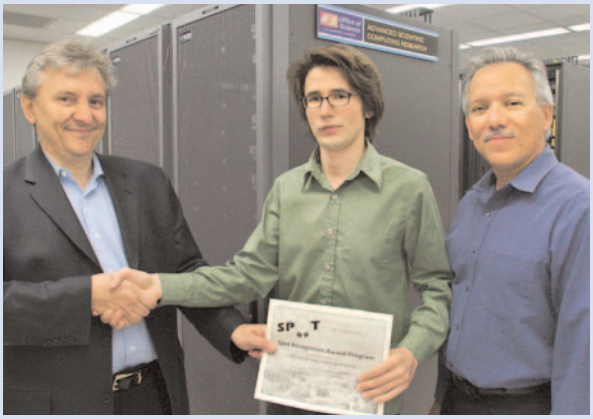
Joshua Schrier Is Newest Alvarez Fellow in Computing Sciences

When Joshua Schrier thinks about how to explain his field of research to his parents, he knows that he won't get far talking about self-consistent fields, wave functions and how the interaction of electrons at the organic-inorganic interface affects the properties in nanocrystals.

So, he tells them he's working on research that could lead to more efficient and less expensive solar cells. As a post-doc in the Computational Research Division's Scientific Computing Group, Schrier is working with Lin-Wang Wang to develop new computational models to study the properties of nanoscale materials.



New Alvarez Fellow Joshua Schrier (center) is congratulated by CRD Director Horst Simon (left) and High Performance Computing Research Department Head Juan Meza.

Schrier, who joined the Lab in May after earning his Ph.D. in chemistry at UC Berkeley, has just been named as the fourth recipient of the Luis Alvarez Computational Science Fellowship. The award honors Nobel Laureate Alvarez, an LBNL physicist who was an early advocate

(continued on page 2)

CRD Staff Making Key Contributions to SC05 Conference in Seattle

When the global HPC community meets at the SC05 conference in Seattle in November, a number of LBNL staff members will be making significant contributions to the conference program. Four of the technical papers accepted by the conference were written principally by CRD staff and two others list LBNL researchers are co-authors.

Here is a list of the papers with LBNL contributions:

"Analyzing Ultra-Scale Application Communication Requirements for a Reconfigurable Hybrid Interconnect," by John Shalf, Shoaib Kamil and Leonid Oliker of CRD and David Skinner of NERSC.

"Leading Computational Methods on Scalar and Vector HEC Platforms," by Leonid Oliker, Michael Wehner and Andrew Canning of CRD, Jonathan Carter of NERSC and others from Princeton Plasma Physics Laboratory, Lawrence Livermore National Laboratory, NEC, Oak Ridge National Laboratory and JAMSTEC.

"Apex-Map: A Global Data Access Benchmark to Analyze HPC Systems and Parallel Programming Paradigms," by Erich Strohmaier and Hongzhang Shan of CRD.

Kathy Yelick, leader of CRD's Future Technologies Group, is an author of "Making Sequential Consistency Practical in Titanium" along with her UC Berkeley students Amir Ashraf Kamil and Jimmy Zhigang Su. Their paper has been nominated for the Best Student Paper Award.

Additionally, Erich Strohmaier is a coauthor with UC San Diego researchers of a paper on "Quantifying Locality in the Memory Access Patterns of HPC Applications."

Mike Welcome of the Future Technologies Group, along with scientists from LLNL, coauthored a paper on "Tera-Scalable Algorithms for Variable-Density Elliptic Hydrodynamics with Spectral Accuracy." More information about the SC05 conference can be found at <http://sc05.supercomputing.org/>.

Joshua Schrier Is Newest Alvarez Fellow in Computing Sciences (continued from p.1)

of using computers to gather and analyze experimental data.

"It's a great honor," said Schrier. Not long after applying for the fellowship, he was browsing at Moe's Books on Berkeley's Telegraph Avenue when he came across a volume of papers by Alvarez, compiled by his fellow researchers. "What was amazing to me was the scope of things he was interested in during his life — from the extinction of dinosaurs to secret chambers in the pyramids to beta decay to the bubble chamber — he did well in many fields, making solid contributions."

Schrier was also impressed by Alvarez' flair for invention. After going on a photo safari in Africa and being bothered by a jittery camera, Alvarez invented a self-stabilizing camera to get clearer shots. "He was always inventing new ways to study problems," Schrier said.

And in the emerging field of nanotechnology, Wang and Schrier are also coming up with new methods for studying problems involving the behavior of electrons, which determine a material's properties. These properties can be used for different purposes, such as processing information. One way of tapping into these properties has been to move the electrons, as is done in transistors. But now scientists are looking into a new idea of controlling the spin of electrons, rather than moving them, to process and store information. If successful, such systems would require less power and would be more robust.

At UC Berkeley, Schrier was a member of a group studying electron spin in semiconductors, as well as working on semiconductor nanocrystals. At the Lab, he is still working on semiconductor nanocrystals, but for different properties, and with different types of quantum mechanical methods. The experimental work is led by LBNL's Paul Alivisatos. His group is growing crystals just a few nanometers in diameter.

"That's the size where an electron really feels trapped, really feels the edges of the structure," Schrier said. Because the electrons behave differently near the edges of such crystals, changing the size of the crystal can change the properties of the material.

In the simplest model of nanocrystals, the electrons live in a "box" with infinitely high walls. It is the confinement produced by these walls that changes the energy levels of the confined electrons. As an example, Schrier uses a violin or guitar string, which makes a sound when a wave vibrates the string. Confining this area of vibration, such as by placing a finger on a fret, changes the frequency of the vibration and the resulting sound. Similarly, by changing the size of an area where electrons live, the energy levels — and properties — can be "tuned."

"There are very intensive experimental projects studying these problems and looking at a wide range of properties and how they scale with size and shape — or how the properties can be tuned," he said. "As we move from the bulk scale down to the atomic level, we find that many assumptions no longer apply. So, we need to start our quantum mechanical description at the atomic level and build the system up from there. This lets us treat problems such as defects, disorder and surface reconstruction in a systematic way."

The standard computational method has been to run long series of calculations of the energy potential of a system, at each step recalculating how the electrons respond to the revised potentials. Finally, at some point, the models results in electrons which are self-consistent, the potential stops changing, and the model for that system is complete.

But Wang has come up with a different, more efficient method of modeling nanosystems. Called "charge patching," the method assumes that the characteristics of a nanosystem are about the same as a bulk system. The method then extracts "motifs," or descriptions of the electron density of the atoms based on their chemical "neighborhood," and moves them around, patching them together to form a good approximation of the actual density.

This approach sidesteps the computationally intensive self-consistency method and, running on a supercomputer at NERSC, produces results in just a few hours. The other method could take weeks to run, Schrier said.

The behavior of electrons at the interface of two materials is of particular interest to members of Alivisatos' group who are looking at developing solar cells by combining nanocrystals with organic polymers. These types of devices would be cheaper than the typical silicon-based solar cells in use today. The idea is that sunlight would excite the polymer, and the excitation would transfer into the nanocrystal and move toward electrodes, generating electricity in the process.

"But we don't have good theoretical models for treating such a system," Schrier said. "Our goal is to come up with better methods based on charge patching so we can improve our understanding of the inorganic-organic interfaces at the nanoscale."

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support for data management and bioinformatics tool development projects at the Joint Genome Institute (JGI), Life Sciences and Physical Biosciences Divisions at LBNL, Biomedical Centers at UCSF, and other similar organizations in the Bay Area.

IMG is accessible to the public at <http://img.jgi.doe.gov/>.